Structures 2+3


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=> d que 192
L14             SCR 475
L16             SCR 2005
L25             STR
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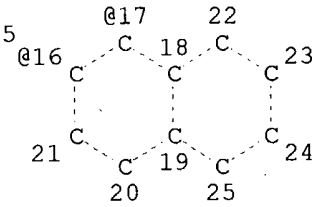
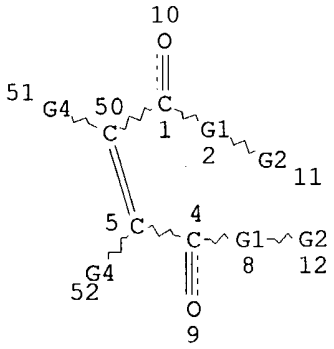
N @13 Ak @14 Cb @15



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VAR G1=O/13
VAR G2=14/15/PH/16/17
VAR G4=H/OH/X/14/15/PH/16/17
NODE ATTRIBUTES:
CONNECT IS E2  RC AT  13
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  15
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  SAT  AT  15
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS X16 C  AT  14
ECOUNT  IS X10 C  AT  15

GRAPH ATTRIBUTES:
RSPEC  16
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE
L27         4617 SEA FILE=REGISTRY SSS FUL L16 AND L14 AND L25
L38              STR
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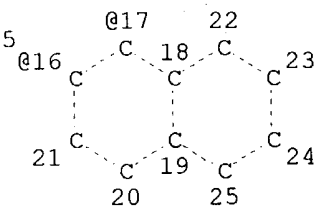
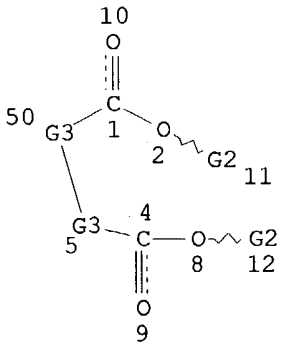
Ak @14 Cb @15





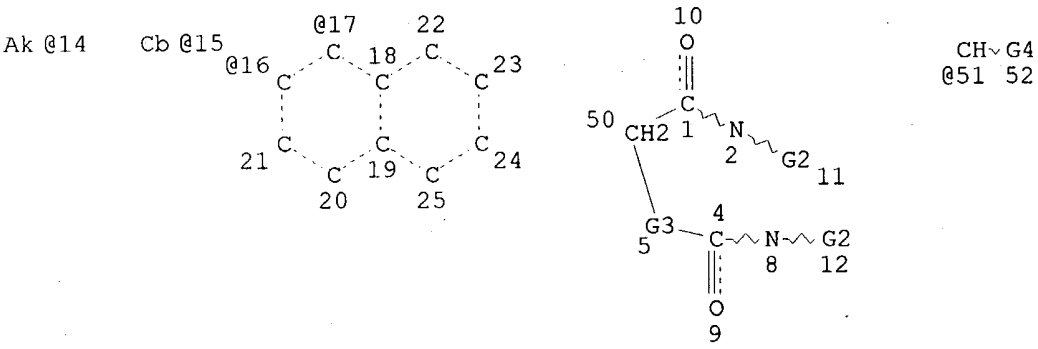
CH~G4
@51 52

G4~C~G4
53 @54 55

VAR G2=14/15/PH/16/17
VAR G3=CH2/51/54
VAR G4=OH/X/14/15/16/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY SAT AT 15
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X16 C AT 14
ECOUNT IS X10 C AT 15

GRAPH ATTRIBUTES:
RSPEC 16
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L42 100 SEA FILE=REGISTRY SUB=L*** SSS FUL L14 AND L16 AND L38
L51 SCR 1993
L54 STR

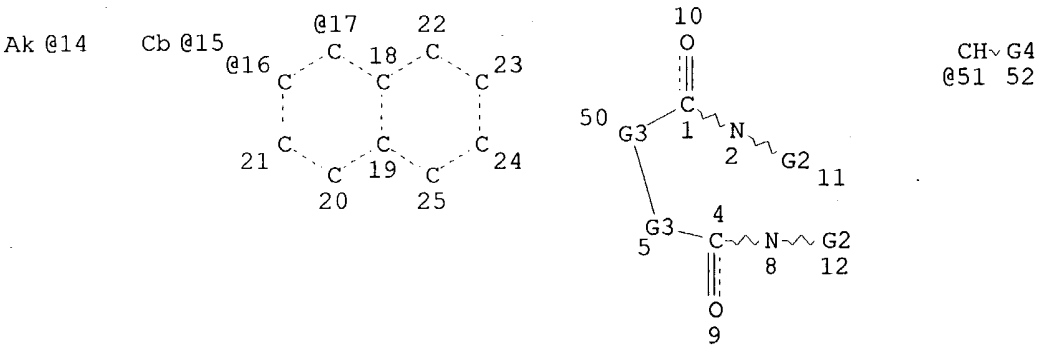


G4~C~G4
53 @54 55

VAR G2=14/15/PH/16/17
VAR G3=CH2/51/54
VAR G4=OH/X/14/15/16/17
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 8
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY SAT AT 15
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X16 C AT 14
ECOUNT IS X10 C AT 15

GRAPH ATTRIBUTES:
RSPEC 16
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L56 142 SEA FILE=REGISTRY SSS FUL L14 AND L16 AND L51 AND L54
L57 STR

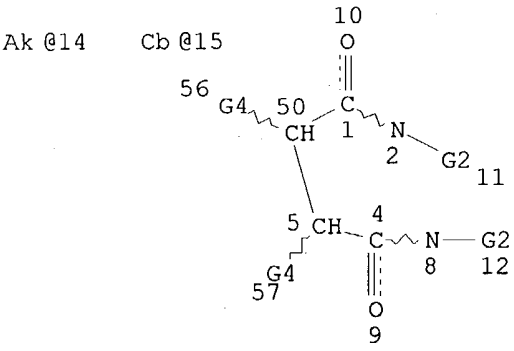


G4 C G4
53 @54 55

VAR G2=14/15/PH/16/17
VAR G3=51/54
VAR G4=OH/X/14/15/16/17
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 8
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY SAT AT 15
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X16 C AT 14
ECOUNT IS X10 C AT 15

GRAPH ATTRIBUTES:
RSPEC 16
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L61 6 SEA FILE=REGISTRY SUB=L*** SSS FUL L57
L75 STR



VAR G2=14/15/PH
VAR G4=OH/X/14/15/PH
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 8
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY SAT AT 15
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X16 C AT 14
ECOUNT IS X10 C AT 15

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
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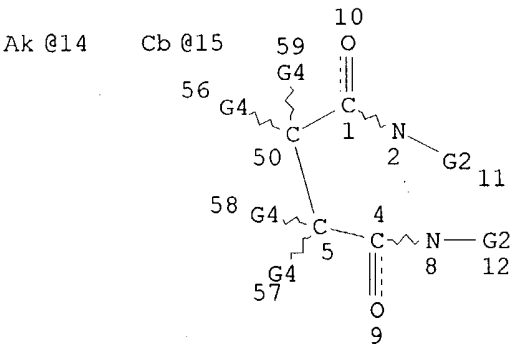
L78 91 SEA FILE=REGISTRY ABB=ON PLU=ON L77/COM
L82 STR



VAR G2=14/15/PH
VAR G4=OH/X/14/15/PH
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 2
CONNECT IS E2 RC AT 8
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 15
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY SAT AT 15
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X16 C AT 14
ECOUNT IS X10 C AT 15

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L84 31 SEA FILE=REGISTRY SSS FUL L14 AND L16 AND L51 AND L82
L88 4986 SEA FILE=REGISTRY ABB=ON PLU=ON L27 OR L42 OR L56 OR L61 OR L78 OR L84
L92 22 SEA FILE=HCAPLUS ABB=ON PLU=ON L88(L)(TOPICAL OR EPIDERM? OR

STRATUM CORN? OR DENDRIT? OR ANTIGEN PRESENT? OR LANGERHAN? OR LYMPH? OR VACCIN? OR ADJUV? OR IMMUNOGEN?)

=> d l92 ibib ab hitind hitstr 1-22

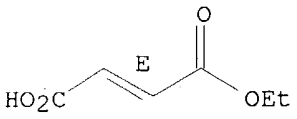
L92 ANSWER 1 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:567900 HCAPLUS
DOCUMENT NUMBER: 138:231660
TITLE: Topical Calcipotriol plus Oral Fumaric Acid Is More Effective and Faster Acting than Oral Fumaric Acid Monotherapy in the Treatment of Severe Chronic Plaque Psoriasis vulgaris
AUTHOR(S): Gollnick, H.; Altmeyer, P.; Kaufmann, R.; Ring, J.; Christophers, E.; Pavel, S.; Ziegler, J.
CORPORATE SOURCE: Department of Dermatology and Venereology, Otto von Guericke University, Magdeburg, Germany
SOURCE: Dermatology (Basel, Switzerland) (2002), 205(1), 46-53
CODEN: DERAEG; ISSN: 1018-8665
PUBLISHER: S. Karger AG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Background: Calcipotriol is an established topical therapy for psoriasis vulgaris. Objective: This study aimed to investigate whether the addn. of calcipotriol to fumaric acid ester (FAE) monotherapy had an additive efficacy and an FAE-sparing effect in patients with severe plaque psoriasis. Methods: This multicenter, randomized, double-blind, vehicle-controlled study included 143 patients for up to 13 wk treatment. Group A received FAE tablets (Fumaderm) with an increasing daily dosage from 105 to 1075 mg + ointment vehicle. Group B received FAE tablets + calcipotriol ointment (50 .mu.g/g). Ointments were applied twice daily. Clin. response was assessed using percentage changes in the Psoriasis Area and Severity Index (PASI), from baseline to treatment end. Results: The mean percentage change in the PASI was -76.1% in group B and -51.9% in group A, the difference between treatments was -24.2% (95% CI from -34.2 to -14.2%; $p < 0.001$). Group B responded more rapidly to treatment. Investigators' and patients' overall efficacy assessments were significantly more favorable for group B (p .ltoreq. 0.001). Group B was prescribed less FAE than group A. This difference was greatest at the last visit (mean daily dose 529 and 685 mg, resp.; $p = 0.006$). Overall adverse events in the two groups were similar. Conclusion: This study shows that the combination of calcipotriol and FAEs is significantly more effective and faster acting than FAE monotherapy in the treatment of severe plaque psoriasis. The combination has a slight FAE-sparing effect and therefore a superior benefit/risk ratio.
CC 1-12 (Pharmacology)
IT 112965-21-6, Calcipotriol **150958-38-6**, Fumaderm
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** calcipotriol plus oral fumaric acid is more effective and faster acting than oral fumaric acid monotherapy in treatment of severe chronic plaque psoriasis vulgaris in humans)
IT **150958-38-6**, Fumaderm
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** calcipotriol plus oral fumaric acid is more effective and faster acting than oral fumaric acid monotherapy in

treatment of severe chronic plaque psoriasis vulgaris in humans)
RN 150958-38-6 HCAPLUS
CN 2-Butenedioic acid (2E)-, dimethyl ester, mixt. with ethyl hydrogen (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 2459-05-4
CMF C6 H8 O4

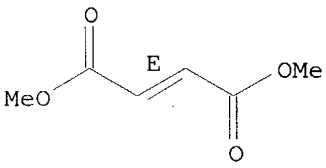
Double bond geometry as shown.



CM 2

CRN 624-49-7
CMF C6 H8 O4

Double bond geometry as shown.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:71815 HCAPLUS
DOCUMENT NUMBER: 136:139823
TITLE: Composition for topically delivering vitamin C
INVENTOR(S): Fitzpatrick, Richard E.; Garruto, John A.
PATENT ASSIGNEE(S): Skinmedica, Inc., USA
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002005751	A1	20020124	WO 2001-US21949	20010712

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1303245	A1	20030423	EP 2001-954655		20010712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
US 2002028844	A1	20020307	US 2001-939400		20010824
US 2003211126	A1	20031113	US 2003-332725		20030110
PRIORITY APPLN. INFO.:			US 2000-614691	A	20000713
			WO 2001-US21949	W	20010712

AB A compn. for the topical application of vitamin C comprising one or more lipid-sol. forms of vitamin C, one or more water-sol. forms of vitamin C and one or more .alpha.-hydroxylated acids. The compn. can also comprise an anhyd. gel, ethoxydiglycol, a lipid-sol. analog of pro-vitamin B-5, .alpha.-bisabolol, and one or more forms of vitamin E.

IC ICM A61K006-00
ICS A61K007-00; A61K031-74; A61K031-34; A01N043-08

CC 63-6 (Pharmaceuticals)

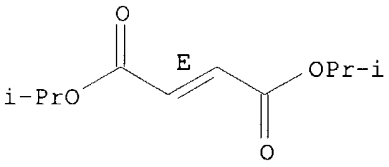
IT 58-95-7, Tocopheryl acetate 81-13-0D, Provitamin B5, analogs 111-90-0 515-69-5, .alpha.-Bisabolol 617-73-2, .alpha.-Hydroxycaprylic acid 1406-18-4, Vitamin e 2984-55-6, .alpha.-Hydroxylauric acid 5393-81-7, Decanoic acid, 2-hydroxy- **7283-70-7**, Diisopropyl fumarate 29710-31-4, Cetyl octanoate 74563-64-7, Phytantriol
RL: MOA (Modifier or additive use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** vitamin C compns.)

IT **7283-70-7**, Diisopropyl fumarate
RL: MOA (Modifier or additive use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** vitamin C compns.)

RN 7283-70-7 HCAPLUS

CN 2-Butenedioic acid (2E)-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	2001:798023 HCAPLUS
DOCUMENT NUMBER:	135:348882
TITLE:	Inorganic polymer-based microcapsules with enhanced formulation stability and delivery of topical active ingredients
INVENTOR(S):	Lapidot, Noa; Magdassi, Shlomo; Avnir, David; Rottman, Claudio; Gans, Orit; Seri-Levy, Alon
PATENT ASSIGNEE(S):	Sol-Gel Technologies Ltd., Israel

SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

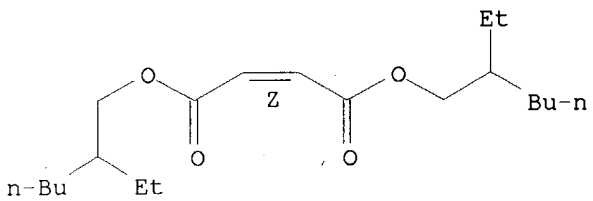
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001080823	A2	20011101	WO 2001-IL370	20010420
WO 2001080823	A3	20030530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2001010600	A	20030415	BR 2001-10600	20010420
EP 1335693	A2	20030820	EP 2001-925838	20010420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003534249	T2	20031118	JP 2001-577923	20010420
US 2002064541	A1	20020530	US 2001-983229	20011023

PRIORITY APPLN. INFO.: US 2000-198749P P 20000421
WO 2001-IL370 W 20010420

AB A therapeutic or cosmetic compn. for topical application, capable of stabilizing an active ingredient and delivering said ingredient, comprising a plurality of microcapsules having a core-shell structure and a diam. of approx. 0.1-100 .mu.. The core of each microcapsule includes at least one active ingredient, and is encapsulated within a microcapsular shell. The shell is comprised of at least one inorg. polymer obtained by a sol-gel process, and the shell protects the active ingredient before topical application and releases the ingredient after topical application. This compn. is useful to encapsulate active ingredients that are unstable in formulation, or are irritating to the skin. The present invention further discloses a process for the encapsulation of an active ingredient in the form of a dispersion within a hydrophobic phase. For example, combinations of erythromycin and benzoyl peroxide are useful in the treatment of acne but usually must be formulated as a two component system because of incompatibility of the two active ingredients. Thus, erythromycin was encapsulated in silica; 1.7 g of erythromycin was mixed with 14.9 g of octylmethoxy cinnamate, and 19.5 g of tetraethoxy silane (TEOS) was added. This oil phase was emulsified and the emulsion was poured into a basic soln. of pH 11.5. The mixt. was stirred at 50-240 rpm. Flocculation was induced by the addn. of MgSO4 at a final concn. of 0.1% by wt. The ppt. was collected by filtration and a product obtained was a paste with a particle size distribution of 1-12 .mu. (an av. size of 6.2 .mu.). Encapsulation of benzoyl peroxide (30 g of 7% soln. in diisopropyl sebacate) was carried out by mixing it with 20 g of TEOS. The org. phase was emulsified in 200 g of an aq. soln. contg. 1% CTAC under high shear. The emulsion obtained was poured into a reactor contg. 200 g NaOH aq. soln. at pH 10 and stirred. The final product was re-suspended in water to obtain a dispersion contg. a 3% benzoyl peroxide encapsulated in silica particles of 0.5015 .mu..

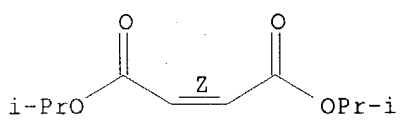
IC ICM A61K009-00
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 62
IT 50-81-7, Vitamin C, biological studies 50-81-7D, Vitamin C, esters and salts 56-81-5, Glycerol, biological studies 58-95-7, Vitamin E acetate 60-00-4, Ethylenediamine tetra acetic acid, biological studies 60-54-8, Tetracycline 65-85-0D, Benzoic acid, C12-15 alkyl esters, biological studies 78-10-4, Tetraethoxysilane 103-23-1, Diethylhexyladipate 110-27-0, Isopropylmyristate 111-90-0, Transcutol 112-02-7, CTAC 112-80-1, Oleic acid, biological studies 114-07-8, Erythromycin 118-60-5, 2-Ethylhexyl salicylate 119-36-8, Methyl salicylate 122-62-3 128-37-0, BHT, biological studies **142-16-5** 1406-18-4, Vitamin E 1429-50-1, Ethylenediamine tetra (methylenephosphonic acid) 1633-00-7, Hexamethylenediamine tetra acetic acid 2787-09-9, Synthomycin 5466-77-3 6938-94-9, Diisopropyladipate 7147-34-4, Bernel ester TOC 7491-02-3, Diisopropylsebacate 7631-86-9, Silica, biological studies 7632-04-4, Sodium perborate 9003-39-8, Polyvinylpyrrolidone 9006-65-9, Dimethicone **10099-70-4**, Diisopropylmaleate 10578-34-4, Stearyl benzoate 15630-89-4, Sodium percarbonate 15827-60-8, Diethylenetriamine penta (methylenephosphonic acid) 18323-44-9, Clindamycin 19666-16-1, Tridecylsalicylate 23605-74-5 25013-16-5, BHA 34364-24-4, Isostearyl benzoate 42557-10-8, Dow Corning 200 108347-89-3 108347-90-6 113973-04-9 114355-44-1 141121-11-1 145686-34-6, Abil EM 90 153190-98-8, Poloxamer 105 benzoate 190085-41-7
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inorg. polymer-based microcapsules with enhanced formulation stability and delivery of **topical** active ingredients)
IT **142-16-5 10099-70-4**, Diisopropylmaleate
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inorg. polymer-based microcapsules with enhanced formulation stability and delivery of **topical** active ingredients)
RN 142-16-5 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

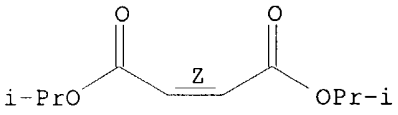
Double bond geometry as shown.



RN 10099-70-4 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.





L92 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:713821 HCAPLUS
DOCUMENT NUMBER: 135:256125
TITLE: Method to enhance the immunogenicity of an antigen
INVENTOR(S): Cowing, Carol O.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. 6,210,672.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2001024649	A1	20010927	US 2001-809158	20010315
US 6210672	B1	20010403	US 1998-176044	19981020
WO 2002074332	A2	20020926	WO 2002-US4752	20020213
WO 2002074332	A3	20030327		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1368057	A2	20031210	EP 2002-723174	20020213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

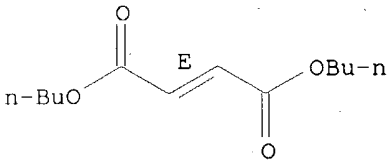
PRIORITY APPLN. INFO.: US 1998-176044 A2 19981020
US 2001-809158 A 20010315
WO 2002-US4752 W 20020213
OTHER SOURCE(S): MARPAT 135:256125
AB The present invention is related to a method for enhancing the immunogenicity of an antigen in a mammal by introducing into the mammal an antigen or a portion thereof and administering to the mammal a topical treatment that increases antigen presentation in a lymphoid organ. The topical treatment comprises a lipophilic mol. capable of traversing the stratum corneum and inducing the immature dendritic cells to migrate to the draining lymphoid organ.
IC ICM A61K039-38
NCL 424184100
CC 15-2 (Immunochemistry)
Section cross-reference(s): 63
IT 65-85-0, Benzoic acid, biological studies 67-64-1, Acetone, biological studies 76-22-2, Camphor 84-62-8, Diphenylphthalate 84-66-2,

Diethylphthalate 84-74-2, Dibutyl phthalate 84-76-4, Dinonylphthalate 85-68-7, Benzylbutylphthalate **105-75-9**, Dibutylfumarate **105-76-0**, Dibutylmaleate 117-81-7, Dioctylphthalate 131-11-3, Dimethylphthalate 131-16-8, Dipropylphthalate **141-02-6** 141-03-7, Dibutylsuccinate **142-16-5**, Di(2-ethylhexyl)maleate 1330-75-2, Diisooctylfumarate 1330-76-3, Diisooctylmaleate **2915-53-9 7242-17-3**, Diphenylmaleate 14491-66-8, Dioctylsuccinate 26545-51-7, N,N-Diethyltoluamide 28553-12-0, Diisononylphthalate 34006-77-4, Ethylmethylphthalate 62563-15-9, Dibutyl D-tartrate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**vaccination** with an antigen and **topical** treatment with a lipophilic mol. that increases the no. of **antigen-presenting dendritic** cells in draining **lymphoid** organs)

IT **105-75-9**, Dibutylfumarate **105-76-0**, Dibutylmaleate **141-02-6 142-16-5**, Di(2-ethylhexyl)maleate **2915-53-9 7242-17-3**, Diphenylmaleate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**vaccination** with an antigen and **topical** treatment with a lipophilic mol. that increases the no. of **antigen-presenting dendritic** cells in draining **lymphoid** organs)

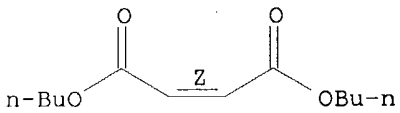
RN 105-75-9 HCAPLUS
CN 2-Butenedioic acid (2E)-, dibutyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



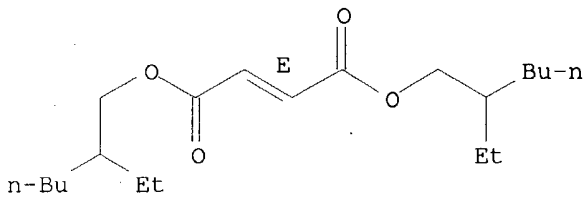
RN 105-76-0 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dibutyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



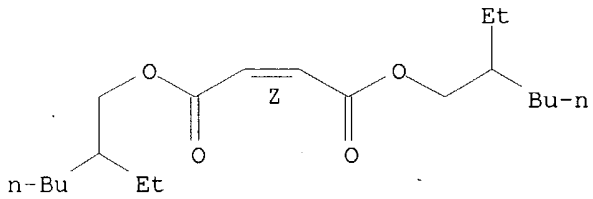
RN 141-02-6 HCAPLUS
CN 2-Butenedioic acid (2E)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



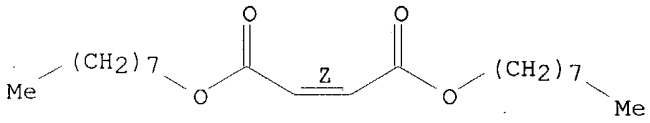
RN 142-16-5 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



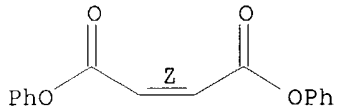
RN 2915-53-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dioctyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 7242-17-3 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diphenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:238058 HCAPLUS
DOCUMENT NUMBER: 134:271240
TITLE: Topical immunostimulation to induce Langerhans cell migration
INVENTOR(S): Cowing, Carol
PATENT ASSIGNEE(S): Torrey Pines Institute for Molecular Studies, USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6210672	B1	20010403	US 1998-176044	19981020
US 2001024649	A1	20010927	US 2001-809158	20010315

PRIORITY APPLN. INFO.: US 1998-176044 A2 19981020
OTHER SOURCE(S): MARPAT 134:271240

AB Disclosed is a method for enhancing an immune response against an antigen by topical administration of an antigen or a portion thereof in conjunction with an enhancer of skin penetration and an inducer of Langerhans cell migration. Complete EG7-OVA tumor-specific immunity was obsd. in mice by intravaginal topical application of 240 .mu.g Ser-Ile-Ile-Asn-Phe-Glu-Lys-Leu in 10 .mu.L dil. DMSO followed by application of 10 .mu.L di-Bu phthalate in acetone 1 h later.

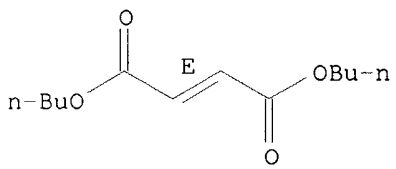
IC ICM A61K039-00
NCL 424184100
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 15

IT 65-85-0, Benzoic acid, biological studies 67-68-5, Dimethylsulfoxide, biological studies 76-22-2, Camphor. 84-62-8, Diphenylphthalate 84-66-2, Diethylphthalate 84-74-2, DiBUtylphthalate 84-76-4, Dinonylphthalate 88-99-3D, 1,2-Benzenedicarboxylic acid, derivs. **105-75-9**, Dibutylfumarate 117-84-0, Dioctylphthalate 131-11-3, Dimethylphthalate 131-16-8, Dipropylphthalate **141-02-6** 141-03-7, Dibutylsuccinate **142-16-5**, Di(2-ethylhexyl) maleate 1330-75-2, Diisooctylfumarate 1330-76-3, Diisooctylmaleate **2915-53-9**, Dioctyl maleate 14491-66-8, Dioctylsuccinate 26545-51-7, N,N-Diethyl-toluamide 27409-39-8 28553-12-0, Diisononylphthalate 62563-15-9, Dibutyl-D-tartrate
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(**topical** immunostimulation to induce **Langerhans** cell migration)

IT **105-75-9**, Dibutylfumarate **141-02-6** **142-16-5**, Di(2-ethylhexyl) maleate **2915-53-9**, Dioctyl maleate
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(**topical** immunostimulation to induce **Langerhans** cell migration)

RN 105-75-9 HCAPLUS
CN 2-Butenedioic acid (2E)-, dibutyl ester (9CI) (CA INDEX NAME)

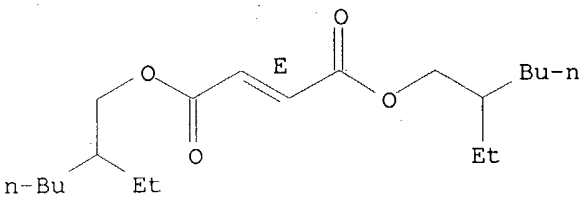
Double bond geometry as shown.



RN 141-02-6 HCAPLUS

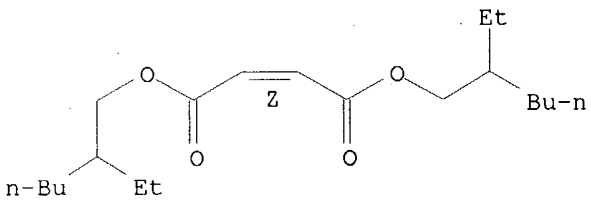
CN 2-Butenedioic acid (2E)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



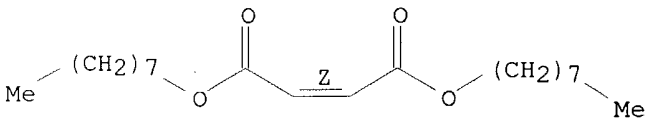
RN 142-16-5 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 2915-53-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dioctyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:666735 HCAPLUS
DOCUMENT NUMBER: 133:238019
TITLE: Preparation of aminopyrimidopyrimidines and related compounds as inhibitors of epidermal growth factor receptor-mediated cell proliferation.
INVENTOR(S): Himmelsbach, Frank; Langkopf, Elke; Blech, Stefan; Jung, Birgit; Metz, Thomas; Solca, Flavio
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055162	A2	20000921	WO 2000-EP2229	20000314
WO 2000055162	A3	20001228		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19911510	A1	20000921	DE 1999-19911510	19990315
EP 1163242	A2	20011219	EP 2000-920498	20000314
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002539214	T2	20021119	JP 2000-605591	20000314
US 2002082420	A1	20020627	US 2001-933597	20010821

PRIORITY APPLN. INFO.: DE 1999-19911510 A 19990315
WO 2000-EP2229 W 20000314

OTHER SOURCE(S): MARPAT 133:238019

AB Title compds. [I; Ra = H, alkyl; Rb = (substituted) Ph, PhCH2, PhCH2CH2; XY = N:C(AB)CH:CH, CH:NC(AB):CH, N:C(AB)N:CH, etc.; A = alkyleneoxy, cycloalkyleneoxy, (substituted) alkyleneimino, cycloalkyleneimino, azetidinylene, piperidinylene, piperazinylene, etc.; B = R6O2CA1NR5, etc.; R5 = H, (substituted) alkyl, cycloalkyl, cycloalkylalkyl; A1 = (substituted) alkylene; R6 = H, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, cycloalkylalkyl, etc.], were prepd. Thus, 4-[(3-chloro-4-fluorophenyl)amino]-6-[[1-[(methoxycarbonyl)methyl]piperidin-4-yl]amino]pyrimido[5,4-d]pyrimidine was stirred with aq. NaOH in THF to give 96% 4-[(3-chloro-4-fluorophenyl)amino]-6-[[1-[(carboxymethyl)methyl]piperidin-4-yl]amino]pyrimido[5,4-d]pyrimidine. I inhibited EGF-dependent proliferation of F/L-HERc cells with IC50 = 7-2510 nM.

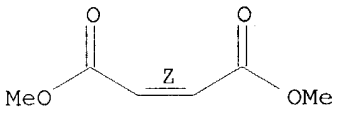
IC ICM C07D487-04
ICS A61K031-519; C07D471-04; A61P035-00; C07D487-04; C07D239-00; C07D239-00; C07D471-04; C07D239-00; C07D221-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 96-32-2, Methyl bromoacetate 96-33-3 96-42-4, 3-Pyrrolidinone 105-36-2, Ethyl bromoacetate 540-51-2, 2-Bromoethanol 620-72-4, Phenyl bromoacetate **624-48-6**, Dimethyl maleate 682-30-4, Diethyl vinylphosphonate 868-26-8, Dimethyl bromomalonate 937-41-7, Phenyl acrylate 1663-39-4 2495-35-4, Benzyl acrylate 3395-91-3, Methyl 3-bromopropionate 5292-43-3, tert-Butyl bromoacetate 5437-45-6, Benzyl bromoacetate 13515-93-0, Sarcosine methyl ester hydrochloride 52605-49-9, Sarcosine ethyl ester hydrochloride 57611-57-1 71879-50-0 73874-95-0, tert-Butyl 4-piperidinylcarbamate 75014-35-6, Glycine, N-(2-hydroxyethyl)-, ethyl ester, hydrochloride 83948-53-2, 3-(tert-Butoxycarbonylamino)propyl bromide 156599-01-8 161975-39-9 176637-10-8 177906-48-8 177907-91-4 182166-44-5, Indan-5-yl acrylate 196512-13-7 196612-11-0 196612-97-2 294181-51-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aminopyrimidopyrimidines and related compds. as inhibitors of **epidermal** growth factor receptor-mediated cell proliferation)

IT **624-48-6**, Dimethyl maleate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aminopyrimidopyrimidines and related compds. as inhibitors of **epidermal** growth factor receptor-mediated cell proliferation)
RN 624-48-6 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:586852 HCAPLUS
DOCUMENT NUMBER: 134:158580
TITLE: Activity of human contact allergens in the murine local lymph node assay
AUTHOR(S): Ryan, C. A.; Gerberick, G. F.; Cruse, L. W.; Basketter, D. A.; Lea, L.; Blaikie, L.; Dearman, R. J.; Warbrick, E. V.; Kimber, I.
CORPORATE SOURCE: The Procter & Gamble Company, Cincinnati, OH, 45253, USA
SOURCE: Contact Dermatitis (2000), 43(2), 95-102
CODEN: CODEDG; ISSN: 0105-1873
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The murine local lymph node assay (LLNA) is a predictive test for the identification of chems. that have the potential to cause skin sensitization. Since its original development, the assay has been the subject of national and international evaluation studies and extensive comparisons with guinea pig tests and human data. On the basis of these investigations, the LLNA has recently been endorsed by ICCVAM (Interagency Coordinating Committee on the Validation of Alternative Methods) as a stand-alone method for skin sensitization hazard identification. At the same time, ICCVAM confirmed that, although the LLNA is not an in vitro method, it does represent a refinement in the way animals are used and can provide a means for reducing the no. of animals used in sensitization hazard assessment. The investigations described here were designed to explore further the ability of the LLNA to identify accurately those chems. that cause allergic contact dermatitis in humans. To that end, the authors have measured, among 3 independent labs., LLNA responses induced by a total of 18 test chems., 11 of which are known to cause skin sensitization and 7 of which are believed not to be assocd. with any significant evidence of allergic contact dermatitis in humans. The LLNA correctly classified 16 of the 18 materials. The 11 chems. tested which are assocd. with allergic contact dermatitis in humans were found to be pos. in the LLNA. Of the 7 materials believed to be non-sensitizers, 5 were neg. in the LLNA and 2 produced pos. results. Collectively, these data provide addnl. evidence that the LLNA is able to discriminate skin sensitizers from those chems. which do not possess a significant skin sensitization potential and thus provides a method for hazard

identification that offers important animal welfare benefits.
CC 4-3 (Toxicology)
Section cross-reference(s): 15
IT 56-81-5, 1,2,3-Propanetriol, biological studies 71-36-3, 1-Butanol, biological studies 78-70-6 84-66-2 99-76-3 100-06-1 104-27-8 110-27-0 111-80-8 122-57-6 122-78-1, Benzeneacetaldehyde **141-05-9** 886-38-4 2892-51-5 5406-12-2 13706-86-0 17369-59-4 25646-71-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (activity of human contact allergens in murine local **lymph** node assay)
IT **141-05-9**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (activity of human contact allergens in murine local **lymph** node assay)
RN 141-05-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:427931 HCAPLUS
DOCUMENT NUMBER: 133:48699
TITLE: Cosmetics containing fumaric acid esters
INVENTOR(S): Haratake, Akinori; Hirotsu, Sachiyo
PATENT ASSIGNEE(S): Kanebo, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000178116	A2	20000627	JP 1998-360628	19981218

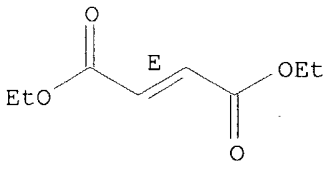
PRIORITY APPLN. INFO.: JP 1998-360628 19981218
AB The present invention relates to cosmetics contg. fumaric acid diesters or monoester salts to strengthen the epidermal barrier functions against environmental causes, such as sunburn. The cosmetic also improves the damaged skin. Application of a soln. contg. 0.5 % di-Me fumarate, caused much less trans-epidermal water loss rate in UV-irradiated hairless mice. A skin lotion contained olive oil 10, iso-Pr myristate 1, polyoxyethylene nonyl Ph ether 0.5, propylene glycol 1, glycerin 2, methylparaben 0.1, ethanol 7, di-Me fumarate 0.5, monoethyl fumarate Ca salt 0.5, distd. water q.s. to 100 %.
IC ICM A61K007-00
CC 62-4 (Essential Oils and Cosmetics)

IT **623-91-6**, Diethyl fumarate **624-49-7**, Dimethyl fumarate
62008-21-3, Monoethyl fumarate zinc salt 62008-22-4, Monoethyl fumarate calcium salt 83918-60-9
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(cosmetics contg. fumaric acid esters to enhance **epidermal** barrier functions)

IT **623-91-6**, Diethyl fumarate **624-49-7**, Dimethyl fumarate
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(cosmetics contg. fumaric acid esters to enhance **epidermal** barrier functions)

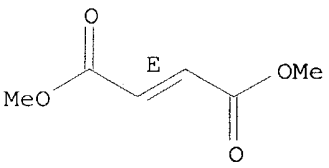
RN 623-91-6 HCAPLUS
CN 2-Butenedioic acid (2E)-, diethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 624-49-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:290803 HCAPLUS
DOCUMENT NUMBER: 132:325812
TITLE: Preparations for topical application of substances having antiandrogenic effect
INVENTOR(S): Kraemer, Karl Theodor; Bohn, Manfred
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000024366	A1	20000504	WO 1999-EP7660	19991012

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,

CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

DE 19848856	A1	20000427	DE 1998-19848856	19981023
DE 19900749	A1	20000713	DE 1999-19900749	19990112
EP 1123082	A1	20010816	EP 1999-953787	19991012
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002528401	T2	20020903	JP 2000-577977	19991012
AU 755165	B2	20021205	AU 2000-10359	19991012
PRIORITY APPLN. INFO.:			DE 1998-19848856 A	19981023
			DE 1999-19900749 A	19990112
			WO 1999-EP7660 W	19991012

OTHER SOURCE(S): MARPAT 132:325812

AB Prepns. contg. .gtoreq.1 physiol. acceptable film-former, .gtoreq.1 physiol. acceptable solvent, .gtoreq.1 plasticizer, and an N-heterocyclic compd. I [R1 = CN, NO2, halo, carboxyalkyl; R2 = CF3, halo, CN; R3 = O, S, NH; X = C:O, C:S; Y = NR4, CR5R6; or XY = R4SC:N; Z = O, CMe2; R4 = H, (substituted) C1-6 alkyl, C2-6 alkenyl; R5 = H, (halo-substituted) C1-4 alkyl; R6 = (substituted) C1-4 alkyl] are useful in the treatment of androgenic alopecia, hirsutism, seborrhea, and acne and can be used in cosmetic products. Thus, a soln. contained 4-[3-(4-hydroxybutyl)-4,4-dimethyl-2,5-dioxo-1-imidazolidinyl]-2-(trifluoromethyl)benzonitrile 5.0, vinylimidazolium methochloride/vinylpyrrolidone copolymer (Luviquat FC 550) 2.5, Cremophor RH 410 2.5, 96% EtOH 63.0, and demineralized water 27.0 wt.%.

IC ICM A61K007-06
ICS A61K009-00; A61K009-70; A61K047-32

CC 62-3 (Essential Oils and Cosmetics)

IT 74-85-1D, Ethylene, polymers with acrylate esters 79-06-1D, Acrylamide, polymers with acrylates 79-10-7D, Acrylic acid, esters, polymers 79-41-4D, Methacrylic acid, esters, polymers 107-18-6D, Allyl alcohol, ethers with pentaerythritol and sugars, polymers with acrylic acid 115-77-5D, Pentaerythritol, allyl ethers, polymers with acrylic acid 9000-07-1, Carrageenan 9000-30-0, Guar gum 9000-30-0D, Guar gum, derivs. 9000-65-1, Gum tragacanth 9003-39-8, PVP 9004-34-6, Cellulose, biological studies 9004-34-6D, Cellulose, derivs., biological studies 9004-61-9, Hyaluronic acid 9005-32-7, Alginic acid 9011-16-9, Methyl vinyl ether/maleic anhydride copolymer 9012-76-4, Chitosan 9012-76-4D, Chitosan, derivs. 9016-00-6D, Dimethylsiloxane, copolyol, phosphopanthenoate 10124-68-2D, N-Octylacrylamide, polymers with acrylates 11138-66-2, Xanthan gum 20404-88-0D, dimethylsiloxane copolyol deriv. 24171-27-5D, 2-Butylaminoethyl methacrylate, polymers with acrylates and octylacrylamide 24937-78-8, Ethylene/vinyl acetate copolymer 25086-89-9 **25119-63-5** 26124-21-0 28211-18-9 30581-59-0D, quaternized 32440-50-9 65829-78-9 76404-21-2 92183-41-0 95144-24-4 96806-20-1 138537-26-5 154992-24-2 203054-83-5, 4-(5-Methyl-2,4-dioxo-5-trifluoromethyl)oxazolidin-3-yl-2-(trifluoromethyl)benzonitrile
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(prepns. for **topical** application of antiandrogenic substances

affecting hair growth)

IT **25119-63-5**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(prepns. for **topical** application of antiandrogenic substances affecting hair growth)

RN 25119-63-5 HCAPLUS

CN 2-Butenedioic acid (2Z)-, dibutyl ester, polymer with methoxyethene (9CI) (CA INDEX NAME)

CM 1

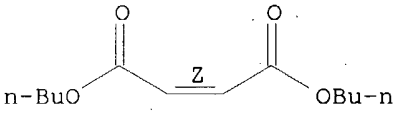
CRN 107-25-5
CMF C3 H6 O

$H_2C{=}CH{-}O{-}CH_3$

CM 2

CRN 105-76-0
CMF C12 H20 O4

Double bond geometry as shown.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:690946 HCAPLUS
DOCUMENT NUMBER: 131:309802
TITLE: Topical immunostimulation to induce Langerhans cell migration
INVENTOR(S): Cowing, Carol O.
PATENT ASSIGNEE(S): Lidak Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9953912	A1	19991028	WO 1998-US7817	19980420

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,

UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2325818	AA	19991028	CA 1998-2325818	19980420
AU 9871324	A1	19991108	AU 1998-71324	19980420
AU 765260	B2	20030911		
EP 1071411	A1	20010131	EP 1998-918392	19980420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002512186	T2	20020423	JP 2000-544317	19980420

PRIORITY APPLN. INFO.: WO 1998-US7817 A 19980420
OTHER SOURCE(S): MARPAT 131:309802

AB Disclosed is a method for enhancing an immune response against an antigen by topical administration of an antigen or a portion thereof in conjunction with an enhancer of skin penetration and an inducer of Langerhans cell migration. The antigen is a tumor-assocd. antigen, and the vaccine compn. is for enhancing immune response against tumor in a mammal.

IC ICM A61K031-12
ICS A61K031-125

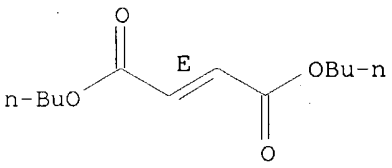
CC 15-2 (Immunochemistry)
Section cross-reference(s): 63

IT 65-85-0, Benzoic acid, biological studies 67-64-1, 2-Propanone, biological studies 67-68-5, DMSO, biological studies 76-22-2, Camphor 84-62-8, Diphenylphthalate 84-66-2, Diethylphthalate 84-74-2, Dibutylphthalate 84-76-4, Dinonylphthalate 85-68-7, Benzylbutylphthalate **105-75-9**, Dibutylfumarate **105-76-0**, Dibutylmaleate 117-81-7, Dioctylphthalate 131-11-3, Dimethylphthalate 131-16-8, Dipropylphthalate **141-02-6** 141-03-7, Dibutylsuccinate **142-16-5**, Di(2-ethylhexyl)maleate 1330-75-2, Diisooctylfumarate 1330-76-3, Diisooctylmaleate **2915-53-9**, Dioctyl maleate **7242-17-3**, Diphenyl maleate 14491-66-8, Dioctylsuccinate 26545-51-7, N,N-Diethyltoluamide 28553-12-0, Diisononylphthalate 34006-77-4, Ethylmethylphthalate 62563-15-9, Dibutyl-D-tartrate 138831-86-4
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical vaccine** comprising lipophilic or org. solvent for stimulating **Langerhans** cell migration and for treating tumor)

IT **105-75-9**, Dibutylfumarate **105-76-0**, Dibutylmaleate **141-02-6 142-16-5**, Di(2-ethylhexyl)maleate **2915-53-9**, Dioctyl maleate **7242-17-3**, Diphenyl maleate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical vaccine** comprising lipophilic or org. solvent for stimulating **Langerhans** cell migration and for treating tumor)

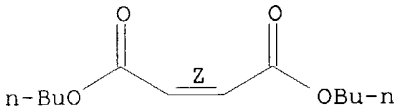
RN 105-75-9 HCAPLUS
CN 2-Butenedioic acid (2E)-, dibutyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



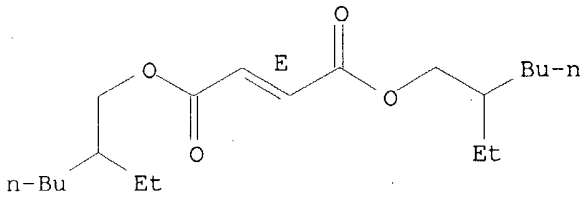
RN 105-76-0 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dibutyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



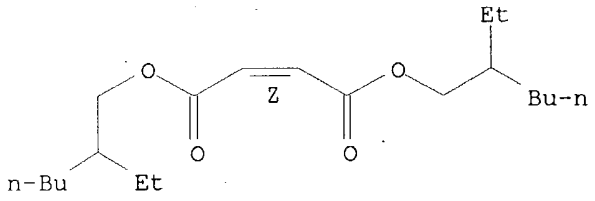
RN 141-02-6 HCAPLUS
CN 2-Butenedioic acid (2E)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



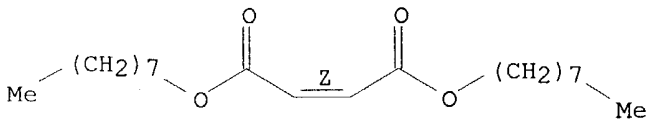
RN 142-16-5 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 2915-53-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dioctyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 7242-17-3 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diphenyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

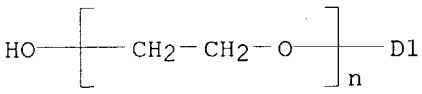
L92 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:537951 HCAPLUS
DOCUMENT NUMBER: 131:140847
TITLE: Adjuvants for pyrethroid insecticide formulations
INVENTOR(S): Killick, Robert William; Killick, Andrew Robert; Wrigley, Peter Ronald; Jones, Peter William
PATENT ASSIGNEE(S): Victorian Chemical International Pty Ltd., Australia
SOURCE: U.S., 19 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5942542	A	19990824	US 1997-997889	19971224
PRIORITY APPLN. INFO.:			AU 1996-5698	19960929

AB A pyrethroid insecticide adjuvant compn. includes alkyl esters of fatty acids, having a level of unsatn. .gtoreq.40%, alkyl esters of dibasic acids, and nonionic emulsifier(s).
IC ICM A01N037-34
ICS A01N053-00
NCL 514521000
CC 5-4 (Agrochemical Bioregulators)
IT 111-62-6, Esterol 123 160759-29-5, Vicchem EOP **189117-52-0**, Vicchem DOP
RL: MOA (Modifier or additive use); USES (Uses)
(**adjuvant** for pyrethroid insecticide formulations)
IT **189117-52-0**, Vicchem DOP
RL: MOA (Modifier or additive use); USES (Uses)
(**adjuvant** for pyrethroid insecticide formulations)
RN 189117-52-0 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester, mixt. with .alpha.-(nonylphenyl)-.omega.-hydroxypoly(oxy-1,2-ethanediyl) and .alpha.-[(9Z)-1-oxo-9-octadecenyl]-.omega.-[[(9Z)-1-oxo-9-octadecenyl]oxy]poly(oxy-1,2-ethanediyl) (9CI) (CA INDEX NAME)

CM 1

CRN 9016-45-9
CMF (C2 H4 O)n C15 H24 O
CCI IDS, PMS

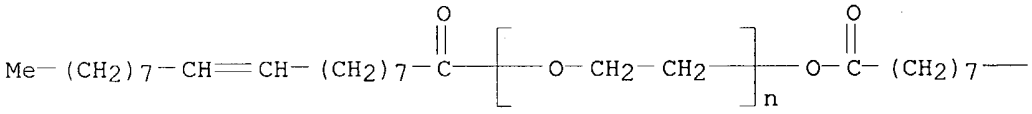


D1— $(CH_2)_8$ —Me

CM 2

CRN 9005-07-6
CMF (C2 H4 O)n C36 H66 O3
CCI PMS

PAGE 1-A



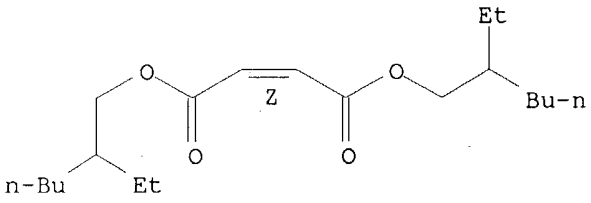
PAGE 1-B

— CH═ CH— $(CH_2)_7$ —Me

CM 3

CRN 142-16-5
CMF C20 H36 O4

Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS

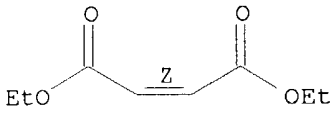
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:485891 HCAPLUS
DOCUMENT NUMBER: 131:268018
TITLE: A comparison of statistical approaches to the derivation of EC3 values from local lymph node assay dose responses
AUTHOR(S): Basketter, David A.; Lea, Linda J.; Dickens, Andrea; Briggs, David; Pate, Ian; Dearman, Rebecca J.; Kimber, Ian
CORPORATE SOURCE: Toxicology Unit, Unilever Research, Safety and Environmental Assurance Centre, Sharnbrook, MK44 1LO, UK
SOURCE: Journal of Applied Toxicology (1999), 19(4), 261-266
CODEN: JJATDK; ISSN: 0260-437X
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Effective risk assessment and management of allergic contact dermatitis require three key factors: adequate hazard identification, measurement of the relative potency of identified hazards and an understanding of the nature, extent and duration of exposure. Suitable methods for hazard identification, such as the murine local lymph node assay (LLNA) and the guinea-pig maximization test, are well established and conditions of human exposure normally can be well anticipated. Thus, the need is for a robust and quant. method for the estn. of relative skin sensitizing potency. One possible approach is via the anal. of LLNA dose-response data. In the LLNA, contact allergens are defined currently as those chems. that cause a threefold or greater increase in lymph node cell proliferative activity compared with concurrent vehicle-treated controls. It is possible to est. the concn. of a sensitizer required to generate a threefold stimulation of proliferation in draining lymph nodes; such a concn. is known as the EC3 value. Using a variety of statistical approaches to derive EC3 values from LLNA dose-response data for 10 chems., it has been demonstrated that simple linear interpolation between the values either side of the threefold stimulation index provides a robust assessment of the EC3 value without the need for recourse to more sophisticated statistical techniques. Provided that the appropriate concns. of test chem. have been selected, EC3 values obtained in this way are reproducible both within and between labs. and form the basis for examn. of the utility of this approach for the estn. of relative skin sensitizing potency.

CC 4-1 (Toxicology)
IT 93-99-2, Phenyl benzoate 97-53-0, Eugenol 97-54-1, Isoeugenol 101-86-0, Hexyl cinnamic aldehyde 109-55-7 **141-05-9** 7778-50-9, Potassium dichromate 15646-46-5, Oxazolone 26172-55-4 30286-29-4
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (comparison of statistical approaches to derivation of EC3 values from local **lymph** node assay dose responses)
IT **141-05-9**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (comparison of statistical approaches to derivation of EC3 values from local **lymph** node assay dose responses)
RN 141-05-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L92 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:603191 HCAPLUS
DOCUMENT NUMBER: 127:253178
TITLE: Topical pharmaceuticals containing metronidazole for the treatment of rosacea and acne
INVENTOR(S): MacKay, Richard; Bourgeau, Jacques D.
PATENT ASSIGNEE(S): Stiefel Canada Inc., Can.
SOURCE: Can. Pat. Appl., 28 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

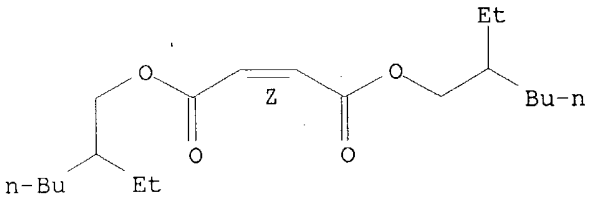
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2161737	AA	19970501	CA 1995-2161737	19951030
CA 2161737	C	19981020		

PRIORITY APPLN. INFO.: CA 1995-2161737 19951030

AB A topical compn. for the treatment of rosacea and acne comprise: (a) an effective amt. of metronidazole (I) or salt thereof; (b) an effective amt. of at least one sunscreen compatible with said metronidazole; (c) a substantially alc. base as a vehicle. A topical gel contg. 1% I and 2% butylmethoxybenozylmethane was applied to patients suffering from rosacea twice daily for nine weeks. The total inflammatory lesion count was reduced by 62% in the treated patients. A topical pharmaceutical contained iso-Pr alc. 71.5250, water 3.6000, dioctyl maleate 5.0000, cyclomethicone 3.0000, octylmethoxy cinnamate 7.5000, isoarachidyl neopentanoate 4.0000, I 1.5000, butylmethoxybenozyl methane 2.0, hydroxypropyl cellulose 1.4000%.

IC ICM A61K031-415
ICS A61K007-40; A61K007-48
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 1
IT 67-63-0, 2-Propanol, biological studies **142-16-5**, Dioctyl maleate 9004-64-2, Hydroxypropyl cellulose 137028-15-0, Isoarachidyl neopentanoate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** pharmaceuticals contg. metronidazole for treatment of rosacea and acne)
IT **142-16-5**, Dioctyl maleate
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**topical** pharmaceuticals contg. metronidazole for treatment of rosacea and acne)
RN 142-16-5 HCAPLUS
CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:315386 HCAPLUS
DOCUMENT NUMBER: 126:289432
TITLE: Insecticide adjuvants for pyrethroids
INVENTOR(S): Killick, Robert William; Killick, Andrew Robert; Wrigley, Peter Ronald; Jones, Peter William
PATENT ASSIGNEE(S): Victorian Chemical International Pty. Ltd., Australia; Killick, Robert William; Killick, Andrew Robert; Wrigley, Peter Ronald; Jones, Peter William
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9712515	A1	19970410	WO 1996-AU603	19960925
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG				
AU 9665835	A1	19970410	AU 1996-65835	19960925
AU 722986	B2	20000817		
AU 9669801	A1	19970428	AU 1996-69801	19960925
EP 854674	A1	19980729	EP 1996-930908	19960925
EP 854674	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1197372	A	19981028	CN 1996-197221	19960925
BR 9610734	A	19990713	BR 1996-10734	19960925
JP 11512725	T2	19991102	JP 1997-513777	19960925
AT 237940	E	20030515	AT 1996-930908	19960925
PRIORITY APPLN. INFO.:			AU 1995-5698 A	19950929
			WO 1996-AU603 W	19960925

AB A pyrethroid insecticide adjuvant compn. includes one or more alkyl esters of fatty acids having a level of unsatn. of .gtoreq.40% or one or more alkyl esters of dibasic acids and nonionic emulsifier. The adjuvants enhance the insecticidal activity of the pyrethroids, mostly by facilitating penetration through the cuticle. Examples are Esterol 123,

Vicchem EOP and Vicchem DOP.

IC ICM A01N025-00
ICS A01N025-02; A01N025-30

CC 5-4 (Agrochemical Bioregulators)

IT 1330-76-3, Diisooctyl Maleate 160759-29-5, Vicchem EOP
189117-52-0, Vicchem DOP
RL: MOA (Modifier or additive use); USES (Uses)
(**adjuvant** for pyrethroids)

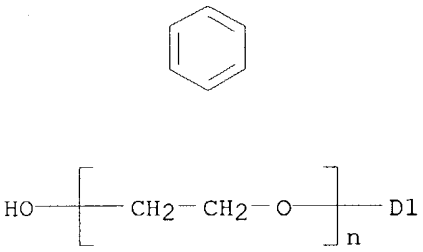
IT **189117-52-0**, Vicchem DOP
RL: MOA (Modifier or additive use); USES (Uses)
(**adjuvant** for pyrethroids)

RN 189117-52-0 HCAPLUS

CN 2-Butenedioic acid (2Z)-, bis(2-ethylhexyl) ester, mixt. with .alpha.-(nonylphenyl)-.omega.-hydroxypoly(oxy-1,2-ethanediyl) and .alpha.-[(9Z)-1-oxo-9-octadecenyl]-.omega.-[[(9Z)-1-oxo-9-octadecenyl]oxy]poly(oxy-1,2-ethanediyl) (9CI) (CA INDEX NAME)

CM 1

CRN 9016-45-9
CMF (C2 H4 O)n C15 H24 O
CCI IDS, PMS

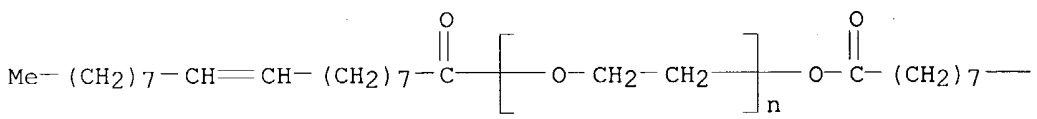


D1-$(CH_2)_8$-Me

CM 2

CRN 9005-07-6
CMF (C2 H4 O)n C36 H66 O3
CCI PMS

PAGE 1-A

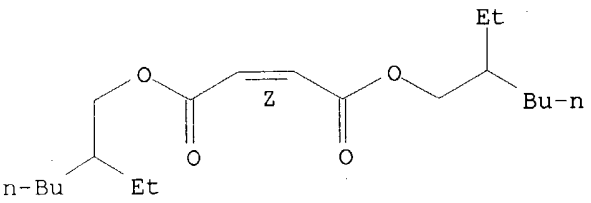


—CH=CH—$(CH_2)_7$—Me

CM 3

CRN 142-16-5
CMF C20 H36 O4

Double bond geometry as shown.



L92 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:299210 HCAPLUS
DOCUMENT NUMBER: 125:26153
TITLE: Effect of fumaric acid, its dimethyl ester, and topical antipsoriatic drugs on epidermal differentiation in the mouse tail model
AUTHOR(S): Sebok, B.; Szabados, T.; Kerenyi, M.; Schneider, I.; Mahrle, G.
CORPORATE SOURCE: Department Dermatology, University Medical School, Pecs, H-7624, Hung.
SOURCE: Skin Pharmacology (1996), 9(2), 99-103
CODEN: SKPHEU; ISSN: 1011-0283
PUBLISHER: Karger
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fumaric acid, fumaric acid di-Me ester, and the dithranol deriv. C4-lactone were studied in the mouse tail test to evaluate their effects on epidermal cell differentiation compared with other topical antipsoriatic drugs, such as betamethasone, calcipotriol, and dithranol. Mouse tails were treated for 2 wk and longitudinal histol. sections prepd. of the tail skin. The length of the orthokeratotic regions (stratum granulosum) was measured on 10 sequential scales per tail and expressed as percentage of the full length of the scale. In addn., epidermal thickness was measured and the efficacy of the various compds. evaluated. In comparison to 2% salicylic acid ointment, all tested compds. except fumaric acid significantly increased the proportion of the orthokeratotic region. C4-lactone and calcipotriol were less effective than dithranol, fumaric acid di-Me ester only moderately influenced cell differentiation, and betamethasone showed the least potent effect. Dithranol was the most potent substance inducing orthokeratosis without increasing epidermal thickness.

CC 1-12 (Pharmacology)

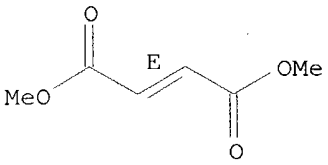
Section cross-reference(s): 63

IT 69-72-7, Salicylic acid, biological studies 110-17-8, Fumaric acid, biological studies 378-44-9, Betamethasone **624-49-7**, Fumaric acid dimethylester 1143-38-0, Dithranol 112965-21-6, Calcipotriol 117566-29-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of fumaric acid, its di-Me ester, and **topical** antipsoriatic drugs on **epidermal** differentiation in the mouse tail model)

IT **624-49-7**, Fumaric acid dimethylester
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of fumaric acid, its di-Me ester, and **topical** antipsoriatic drugs on **epidermal** differentiation in the mouse tail model)

RN 624-49-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:78283 HCAPLUS
DOCUMENT NUMBER: 116:78283
TITLE: Induction of NAD(P)H:quinone reductase in human peripheral blood lymphocytes
AUTHOR(S): Gordon, Gary B.; Prochaska, Hans J.; Yang, Lynda Y. S.
CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA
SOURCE: Carcinogenesis (1991), 12(12), 2393-6
CODEN: CRNGDP; ISSN: 0143-3334
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The induction of quinone reductase [QR; NAD(P)H:(quinone acceptor) oxidoreductase; EC 1.6.99.2] in cultured cells and animal tissues of rodents has provided useful information on mechanisms of protection against carcinogens. The authors have developed a simple and efficient microtiter plate assay for the direct measurement of QR basal activity and inducibility in human peripheral blood lymphocytes (unstimulated, mitogen-stimulated, and Epstein-Barr virus-transformed) grown in suspension culture. In these cells, QR was induced by monofunctional (electrophilic) inducers (i.e. 1,2-dithiole-3-thione, di-Me fumarate, and Me vinyl sulfone) but not by bifunctional inducers (i.e. 1,1'-azonaphthalene, .beta.-naphthoflavone, 2,3,7,8-tetrachlorodibenzo-p-dioxin). QR is a major enzyme of xenobiotic metab. that carries out obligatory two-electron redns. and thereby protects cells against the

toxicity of quinones. It is induced in many tissues coordinately with other enzymes that protect against electrophiles. Since lymphocytes can be sampled easily and repetitively in man, this system may provide a simple short-term marker for assessing the capacity of tissues to detoxify electrophiles, such as quinones, and for measuring the response to inducers.

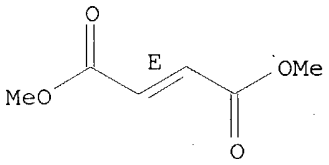
CC 4-6 (Toxicology)
Section cross-reference(s): 1

IT 487-10-5, 1,1'-Azonaphthalene 534-25-8, 1,2-Dithiole-3-thione **624-49-7**, Dimethyl fumarate 1746-01-6, TCDD 3680-02-2, Methyl vinyl sulfone 6051-87-2, .beta.-Naphthoflavone
RL: BIOL (Biological study)
(NAD(P)H:quinone reductase of human **lymphocytes** induction by)

IT **624-49-7**, Dimethyl fumarate
RL: BIOL (Biological study)
(NAD(P)H:quinone reductase of human **lymphocytes** induction by)

RN 624-49-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:580728 HCAPLUS
DOCUMENT NUMBER: 111:180728
TITLE: Topical pharmaceuticals for the treatment of psoriasis containing fumarate esters
INVENTOR(S): Lekim, Dac
PATENT ASSIGNEE(S): Pearson und Co. (G.m.b.H. und Co.), Fed. Rep. Ger.
SOURCE: Ger. Offen., 2 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3728188	A1	19890309	DE 1987-3728188	19870824

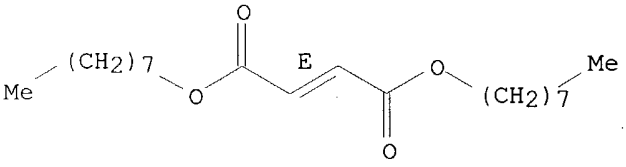
PRIORITY APPLN. INFO.: DE 1987-3728188 19870824
OTHER SOURCE(S): CASREACT 111:180728

AB Fumarate esters are used for the external treatment of psoriasis; such formulations contain 0.5-10.0% esters of fumaric acid with C>2-alcs. and have the form of creams, salves, lotions, body oils. Fumaric acid 100g was dissolved in 500 mL iso-PrOH and treated with 10 mL conc. HCl and refluxed to give 60 g diisopropyl fumarate (I). A salve contained 30 g I and 970 g salve base; the compn. did not give rise to erythema and could be used for the treatment of psoriasis.

IC ICM A61K031-22

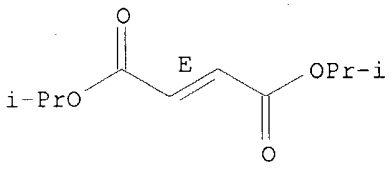
CC 63-6 (Pharmaceuticals)
IT **2997-85-5,** Dioctyl fumarate **7283-70-7,** Diisopropyl fumarate
RL: BIOL (Biological study)
(**topical** pharmaceuticals for psoriasis treatment contg.)
IT **2997-85-5,** Dioctyl fumarate **7283-70-7,** Diisopropyl fumarate
RL: BIOL (Biological study)
(**topical** pharmaceuticals for psoriasis treatment contg.)
RN 2997-85-5 HCAPLUS
CN 2-Butenedioic acid (2E)-, dioctyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 7283-70-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:487553 HCAPLUS
DOCUMENT NUMBER: 109:87553
TITLE: Evaluation of a genotoxicity test measuring DNA-strand breaks in mouse lymphoma cells by alkaline unwinding and hydroxyapatite elution
AUTHOR(S): Garberg, Per; Aakerblom, Eva Lena; Bolcsfoldi, George
CORPORATE SOURCE: AB Astra, Sodertalje, S-151 85, Swed.
SOURCE: Mutation Research (1988), 203(3), 155-76
CODEN: MUREAV; ISSN: 0027-5107
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A rapid genotoxicity test, based on the measurement of the proportion of single- to double-stranded DNA by alk. unwinding and hydroxyapatite elution in mouse lymphoma cells treated in vitro with various chems., was evaluated. Seventy-eight compds. from diverse chem. groups, including commonly tested mutagens, toxic compds. not usually tested for genotoxicity, and nontoxic compds. not thought to be genotoxic, were tested. The results obtained were compared with those from the mouse lymphoma thymidine kinase (TK) locus forward-mutation assay, providing a basis for assessing the relative sensitivity of the 2 assays using the

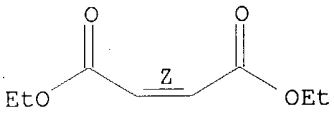
same cells exposed to chems. under similar conditions. Clear evidence of DNA-damaging activity was obtained with 43 of the compds., whereas 4 gave equivocal results. Of the remaining 31 compds., 14 were toxic without inducing DNA damage whereas the rest were nontoxic and did not induce any DNA damage. Results were available from both the alk. unwinding assay and the mouse lymphoma assay for 61 compds.; they showed a concordance between the 2 assays of 77%. Of the 47 compds. that were pos. or equivocal in the alk. unwinding assay, only CCl4 and prednisolone were neg. in the mouse lymphoma assay, whereas 12 of the 19 compds. that were neg. in the alk. unwinding assay were pos. in the mouse lymphoma assay. These included 3 compds. that interfere with nucleic acid metab., and 3 crosslinking agents, which would be expected to produce mutations to a greater extent than strand breaks. The other 6 compds. were anthranilic acid, benzoquinone, p-chloroaniline, di-Et maleate, glucose, and procarbazine-HCl. Of these, only the last is a known carcinogen. There was good overall agreement between the results of the DNA alk. unwinding and mouse lymphoma TK locus assays, but the sensitivity of the alk. unwinding assay is lower for some classes of compds. Bearing this in mind, the alk. unwinding assay is considered suitable as a rapid screen for genotoxic activity in eukaryotic cells.

CC 4-1 (Toxicology)
Section cross-reference(s): 1, 2

IT 50-00-0, Formaldehyde, biological studies 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-32-8, Benzo[a]pyrene, biological studies 50-44-2, 6-Mercaptopurine 50-76-0, Actinomycin D 50-99-7, Glucose, biological studies 51-61-6, 3-Hydroxytyramine, biological studies 56-23-5, Carbon tetrachloride, biological studies 56-53-1 56-57-5, 4-Nitroquinoline-N-oxide 57-13-6, Urea, biological studies 57-97-6 59-05-2, Methotrexate 60-00-4, Ethylenediaminetetraacetic acid, biological studies 60-18-4, L-Tyrosine, biological studies 62-50-0, Ethyl methanesulphonate 62-53-3, Aniline, biological studies 63-68-3, L-Methionine, biological studies 64-17-5, Ethyl alcohol, biological studies 66-22-8, Uracil, biological studies 66-27-3, Methyl methanesulphonate 66-81-9, Cycloheximide 71-43-2, Benzene, biological studies 73-22-3, L-Tryptophan, biological studies 75-07-0, Acetaldehyde, biological studies 86-00-0, 2-Nitrobiphenyl 86-30-6, N-Nitrosodiphenylamine 86-54-4, Hydralazine 86-73-7, Fluorene 90-04-0, o-Anisidine 90-45-9, 9-Aminoacridine 92-52-4, Biphenyl, biological studies 94-59-7, Safrole 99-56-9, 4-Nitro-o-phenylenediamine 100-44-7, Benzyl chloride, biological studies 100-75-4, N-Nitrosopiperidine 104-94-9, p-Anisidine 106-47-8, p-Chloroaniline, biological studies 106-51-4, biological studies 106-89-8, Epichlorohydrin, biological studies 107-22-2, Glyoxal 108-95-2, Phenol, biological studies 110-89-4, Piperidine, biological studies 118-92-3, Anthranilic acid 120-12-7, Anthracene, biological studies 120-80-9, Catechol, biological studies 123-11-5, 4-Methoxybenzaldehyde, biological studies 123-30-8, p-Aminophenol 127-07-1, Hydroxyurea 129-00-0, Pyrene, biological studies **141-05-9**, Diethylmaleate 141-90-2, Thiouracil 143-33-9, Sodium cyanide 144-49-0 147-84-2, biological studies 154-23-4, Catechol 302-01-2, biological studies 443-48-1, Metronidazole 452-06-2, 2-Aminopurine 607-57-8, 2-Nitrofluorene 610-49-1, 1-Aminoanthracene 613-13-8, 2-Aminoanthracene 614-00-6, N-Nitroso-N-methylaniline 630-60-4, Ouabain 671-16-9 759-73-9, N-Ethyl-N-nitrosourea 1074-12-0, Phenylglyoxal 1397-94-0, Antimycin A 3105-97-3, Hycanthone 3483-12-3, Dithiothreitol 5307-14-2, 2-Nitro-p-phenylenediamine 7632-00-0, Sodium nitrite 7647-14-5, Sodium chloride, biological studies

7722-84-1, Hydrogen peroxide, biological studies 9002-93-1, Triton X-100
11097-69-1, Aroclor 1254 15663-27-1, Cis-Diamminedichloroplatinum (II)
25413-64-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(genotoxicity of, in **lymphoma** cells, detn. of, by alk.
unwinding and hydroxyapatite elution)
IT **141-05-9**, Diethylmaleate
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(genotoxicity of, in **lymphoma** cells, detn. of, by alk.
unwinding and hydroxyapatite elution)
RN 141-05-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:55750 HCAPLUS
DOCUMENT NUMBER: 106:55750
TITLE: The effect of adjuvants on the colonic absorption of cefmetazole and [Asu1,7]-eel calcitonin in rats: concentration dependent absorption pathways
AUTHOR(S): Nishihata, Toshiaki; Miyake, Masatoshi; Takahata, Hideo; Kamada, Akira
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: International Journal of Pharmaceutics (1986), 33(1-3), 89-97
CODEN: IJPHDE; ISSN: 0378-5173
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Rat colonic absorption of cefmetazole (I) [56796-20-4] and [Asu1,7]-eel calcitonin (II) [60731-46-6] was enhanced by coadministration of Na salicylate [54-21-7], di-Na EDTA [139-33-3], di-Et ethoxymethylenemalonate (DEEMM) [87-13-8] or trifluoperazine [117-89-5]. Colonic absorption of I and II, enhanced by various concns. of either EDTA or trifluoperazine, appeared to occur via a paracellular pathway. Di-Et maleate [**141-05-9**] did not enhance colonic absorption of II, but it did significantly enhance colonic absorption of I, demonstrating the importance of a paracellular absorption pathway for II. Although low concns. of DEEMM and salicylate enhanced the colonic absorption of only I (having a low mol. wt. of 471), those **adjuvants** at high concns. remarkably enhanced the colonic absorption of both I and the macromol. peptide, II (mol. wt. 3363). This observation suggests two different **adjuvant** mechanisms, depending on the concn. of the **adjuvant**.
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 1, 2

L92 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:115960 HCAPLUS
DOCUMENT NUMBER: 104:115960

TITLE: Possible mechanism regulating barrier function of rat intestinal mucosa against permeation of cefmetazole, a hydrophilic drug
AUTHOR(S): Nishihata, Toshiaki; Takahata, Hideo; Kamada, Akira
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Pharmaceutical Research (1985), (6), 307-9
CODEN: PHREEB; ISSN: 0724-8741
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The nonsurfactant **adjuvants** diethyl maleate (DEM) [**141-05-9**] and diethyl ethoxymethylenemalonate (DEEMM) [87-13-8] enhanced the colonic absorption of the hydrophilic drug cefmetazole (I) [56796-20-4] as I Na salt in rats and concomitantly decreased the nonprotein sulfhydryl concn. of colonic tissue. To test further an assocn. between nonprotein sulfhydryl concn. and membrane permeability, the effects of several **adjuvants**, DEM, DEEMM, EtOH [64-17-5] and Na salicylate [54-21-7], were tested in the everted sac prepn. of rat colon and jejunum. There was a good correlation between decreased nonprotein sulfhydryl concn. and enhanced I absorption in both tissues. Moreover, the addn. of cysteamine [60-23-1] reversed the effects of each **adjuvant** on nonprotein sulfhydryls and I absorption. Thus, tissue levels of nonprotein sulfhydryls regulate, at least in part, the intestinal membrane permeability.
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 1

L92 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:162762 HCAPLUS
DOCUMENT NUMBER: 94:162762
TITLE: Additives enhancing topical corticosteroid action
INVENTOR(S): Van Scott, Eugene J.; Yu, Ruey J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4246261	A	19810120	US 1979-65332	19790809

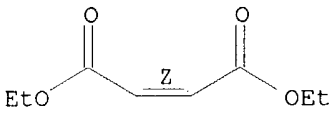
PRIORITY APPLN. INFO.: US 1979-65332 19790809
AB The therapeutic efficacy of corticosteroids in topical treatment of psoriasis, eczema, seborrheic dermatitis, and other inflammatory skin conditions can be greatly enhanced by adding various hydroxy acids in small amts. The addn. of 0.2% atrolactic acid [515-30-0], gluconolactone [90-80-2] or mandelic acid [90-64-2], to a cream contg. 0.2% hydrocortisone 21-acetate [50-03-3] enhanced remission of lesions in the psoriatic patients tested. A combination of hydrocortisone [50-23-7] with mandelic acid or Et pyruvate [617-35-6] was most effective in eradicating the lesions of psoriasis completely.
IC A01N045-00; A61K031-56
NCL 424240000
CC 63-6 (Pharmaceuticals)
IT 50-21-5, biological studies 76-30-2 77-92-9, biological studies 79-14-1, biological studies 87-69-4, biological studies 87-73-0

90-64-2 90-80-2 110-16-7, biological studies 127-17-3, biological studies **141-05-9** 142-45-0 156-06-9 300-85-6 389-36-6
473-81-4 488-31-3 498-36-2 504-33-6 515-30-0 526-84-1 526-95-4
526-99-8 594-61-6 599-04-2 600-15-7 600-22-6 611-73-4 617-35-6
624-48-6 685-73-4 762-21-0 762-42-5 828-01-3 923-11-5
1112-33-0 1113-60-6 1198-69-2 1603-79-8 2381-08-0 2782-07-2
3913-50-6 4026-18-0 6556-12-3 6915-15-7 13100-82-8 13382-27-9
15206-55-0 23351-51-1 32449-92-6 77228-68-3 77340-56-8
RL: BIOL (Biological study)
(corticosteroid **topical** compns. contg., for enhanced activity)

IT **141-05-9 624-48-6**
RL: BIOL (Biological study)
(corticosteroid **topical** compns. contg., for enhanced activity)

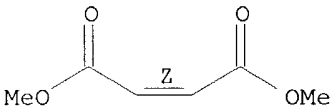
RN 141-05-9 HCAPLUS
CN 2-Butenedioic acid (2Z)-, diethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 624-48-6 HCAPLUS
CN 2-Butenedioic acid (2Z)-, dimethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L92 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:164226 HCAPLUS
DOCUMENT NUMBER: 88:164226
TITLE: Effects of diethyl maleate on aryl hydrocarbon hydroxylase and on 3-methylcholanthrene-induced skin tumorigenesis in rats and mice
AUTHOR(S): Chuang, A. H. L.; Mukhtar, Hasan; Bresnick, Edward
CORPORATE SOURCE: Dep. Biochem., Univ. Vermont Coll. Med., Burlington, VT, USA
SOURCE: Journal of the National Cancer Institute (1940-1978) (1978), 60(2), 321-5
CODEN: JNCIAM; ISSN: 0027-8874
DOCUMENT TYPE: Journal
LANGUAGE: English
AB **Topical** administration of diethyl maleate (DEM) [**141-05-9**] and L-methionine sulfoximine (MS) [15985-39-4] reduced the L-glutathione (GSH) [70-18-8] levels in kidneys, livers, and skin of inbred BALB/c mice. **Topical** administration of DEM to BALB/c mice also increased the latency period before development of skin tumors

induced by 3-methylcholanthrene [56-49-5] painting. Similar treatment with MS also increased the latency period, though the delay was not as striking as that obsd. after DEM administration. Furthermore, DEM, which was believed to be specific in its action in reducing tissue GSH, was also capable of inhibiting aryl hydrocarbon hydroxylase (AHH) [9037-52-9] both in vitro and in vivo. Cyclohexene sulfide [286-28-2], another "specific" inhibitor of GSH transferase, inhibited AHH activity as well. Accordingly, the blockade of AHH by DEM may have been partly responsible for the increased latency time in the skin tumorigenesis expts.

CC 1-5 (Pharmacodynamics)
Section cross-reference(s): 4